

3-Methyl-1-phenyl-1H-pyrazol-5-amine  
1131-18-6 | DTXSID6044517

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 55.2 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.58e-01

Confidence level: 9.12e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Urea, N'-(3-chlorophenyl)-N,N-dimethyl-</div> <div>Measured: 61.7</div> <div>Predicted: 54.0</div>	<div>Image not found</div> <div>Urea, 3-(m-methoxyphenyl)-1,1-dimethyl-</div> <div>Measured: 52.5</div> <div>Predicted: 45.4</div>	<div>Image not found</div> <div>Monuron</div> <div>Measured: 89.1</div> <div>Predicted: 79.6</div>
<div>Image not found</div> <div>Urea, N,N-dimethyl-N'-(4-methylphenyl)-</div> <div>Measured: 32.4</div> <div>Predicted: 36.8</div>	<div>Image not found</div> <div>N'-(3,5-Dimethylphenyl)-N,N-dimethylurea</div> <div>Measured: 53.7</div> <div>Predicted: 61.4</div>	